Tiny reversible rearrangement transitions in granular systems

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Abstract

Very dense bidimensional systems of inelastic hard disks excited from the base are studied by means of Newtonian event driven molecular dynamics. A stationary regime is reached where almost perfect crystallographic order is present in the system. When the energy injection is varied in a wide range the center of mass of the system varies smoothly except that at some points it suffers abrupt changes. There are at least two different types of changes and both show hysteresis as if it were a first order transition.

Key words: granular materials, phase transitions, hysteresis
PACS: 81.05.Rm, 05.70.Fh **Published in Physica A, 371 37 (2006)**

Almost a decade ago it was argued that a granular system weakly excited by a vertically vibrating base presents a Fermi-like density profile as a function of height (Hayakawa Hong). For a bidimensional system of N hard inelastic disks, of diameter σ in a box of width $L_x = N_x\sigma$, the proposed form of the linear number density ϕ—normalized to $\int_0^\infty \phi\, dz = N/N_x$—is

$$\phi(z) = \frac{1}{1+\exp\left[\beta(z-z_0)\right]}\,, \qquad z_0(\beta^{-1}) = \frac{1}{\beta}\ln\left(e^{\beta N/N_x}-1\right) \qquad (1)$$

where z is the dimensionless vertical coordinate. The height $z_0(\beta^{-1})$, playing the role of a chemical potential, is the dimensionless position of the superficial layer in the sense that $d^2\phi/dz^2$ vanishes at $z = z_0$. It tends to N/N_x as $\beta \to \infty$. The authors assume that β is connected with the product of the amplitude and the frequency of the vibrating base, $\beta^{-1} \propto (A\omega)^2$ but this is debatable. Their $T \sim \beta^{-1}$ should be directly connected with the temperature of Edwards thermodynamics of granular systems (Edwards et al.).

Starting basically from the first article cited above the authors of (Fiscina Caceres) have made an interesting theoretical and experimental study of the behaviour of the upper layer of these systems.

It is easy to prove that from Eq. (1) the height h of the center of mass, $h = \frac{N_x}{N} \int_0^\infty z\,\phi\,dz$, for large β (small excitation) is $h = N_x/2N + dh$ where

$$dh = \frac{\pi^2 \sigma N_x}{6N} \beta^{-2} + O\left(\beta^{-4}\right) \tag{2}$$

This expresion says that $dh \propto T^2$ but it is not clear what T is. We interprete (Huntley) as implying that $T \propto (A\omega)^{4/3}$ even though this is not stated in that reference. In the following we make no attempt to define T but use as control parameter the temperature T_b associated to the base and find that $dh \propto T^b$ with $0.2 \le b < 0.3$.

* * *

The present article exhibits results obtained from molecular dynamics of bidimensional systems of inelastic hard disks excited by a stochastic still base characterized by a *temperature* T_b. Namely, a particle P hitting the base bounces back as if P were replaced by an independent particle coming from a heat bath (with $T = T_b$) on the other side of the wall. Similar results have also been obtained using a tapping algorithm characterized by a base which induces collisions as if it were moving at constant velocity v_0.

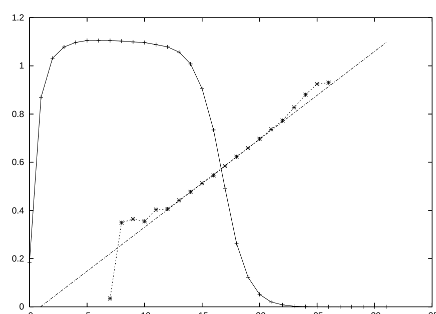

Fig. 1. The figure illustrates a molecular dynamics observation in which the density profile does not show a Fermi-like shape. The reason is that the *granular* temperature is highly inhomogeneous. The secondary curve, to which a straight line has been adjusted, represents $[\log(d/dz(1/\phi))]$ which, for a Fermi distribution, should be a straight line.

The density profile: Since the system is inelastic the kinetic energy per particle (*granular temperature* from now on) is a steep function $T(z)$ which initially decays exponentially. This is the reason for which we do not generally observe a density $\phi(z)$ monotonically decreasing with z but rather a density that at first grows with z, then flattens and finally falls to zero very much like the Fermi distribution described in Eq. (1). We check that $\left[\log\left(\frac{d}{dz}\frac{1}{\phi}\right)\right]$ is a straight line in the upper layer where the density is dropping to zero, as shown in Fig. 1. Such non-monotonic profiles can be produced introducing some modifications into Fermi's function $\phi(z)$: replace $T \sim \beta^{-1}$ by a steep function of z and modifying the purely gravitational energy used in (Hayakawa Hong) introducing a kinetic energy contribution as well. Such profiles will be derived in a forthcoming article (Risso Cordero). If the degree of excitation of the system is low enough the observed density profile does decrease monotonically with height.

Height of the center of mass and its discontinuities: In our simulations we observe the behavior of h as a function of T_b. We do this for a system of $N = 512$ inelastic hard disks of diameter $\sigma = 1$, mass $m = 0.25$ and under gravity $g = 1$ (with these choices any other quantity is dimensionless). The box has witdth $L_x = 29$; the disks have translational and rotational degrees of freedom and the collision rule has been described in (Risso et al.). The values of the normal and tangential restitution coefficients are set to 0.9 and both (static and dynamic) friction coefficients are set to 0.2. We start the simulation with a temperature T_b that is kept fixed until the system is fully relaxed, then T_b is slightly changed and, starting from the last state, the simulation proceeds relaxing the system again. This is done both increasing and decreasing T_b and covering a wide range of temperatures.

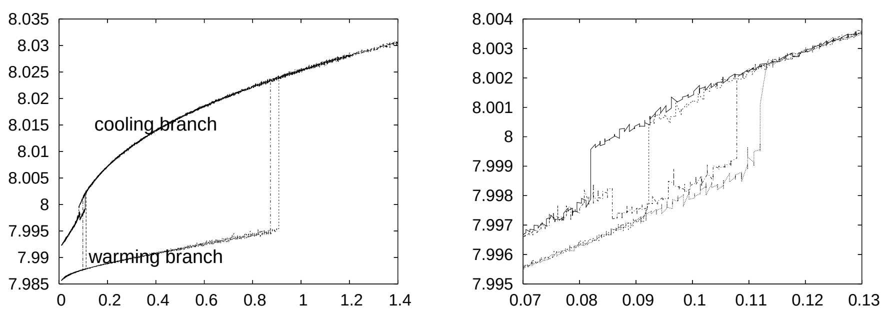

Fig. 2. The system of very cold inelastic disks can show tiny discontinuities in the height h of the center of mass, as the energy input T_b varies. The left graph is dominated by two cicles of hysteresis: one which has its jumps at about $T_b \approx 0.1$ and $T_b \approx 0.9$ and the other one, so tiny that it is almost invisible at left, which is enlarged in the graph at right. The figure at right really shows several transitions from a higher (warmer) state to at least three different lower (cooler) states. The warmer state has crystallographic order while the cooler states present zig-zag rearrangement of the grains as shown in Fig. 3

The graph in Fig. 2 represents $h(T_b)$ when the simulation goes down and up twice over the whole range (namely each T_b is visited four times). In the first downward path the height h has a discontinuity just below $T_b = 0.1$. Later, when T_b starts going up, h takes the same values and goes on increasing continuously well beyond $T_b = 0.1$. Only near $T_b = 0.9$ it jumps up *recovering the* *values it had* coming down. The first hysteretic cycle has been closed. It has to be strongly emphasized that the system recovers previous values after a discontinuous jump up. This means that the jump down is not a mere reordering because in that case it would remain in that more compact configuration until it changes to a more "disordered state", when T_b is increased, it would end in *any* disordered state. Recovering the same less compact order has a meaning which one could perhaps relate, generalizing concepts of thermodynamics, to minimal free energy and/or entropy. More comments on this later on.

The coolong branch in the graph at left in Fig. 2 can be adjusted, in the range $0.2 \leq T_b \leq 0.5$, to $h(T_b) \approx 7.97 + 0.0535\, T_b^{1/4}$.

The next time T_b comes down it makes a smaller transition and again it presents hysteresis. This is the tiny transition shown in the right graphs in Fig. 2.

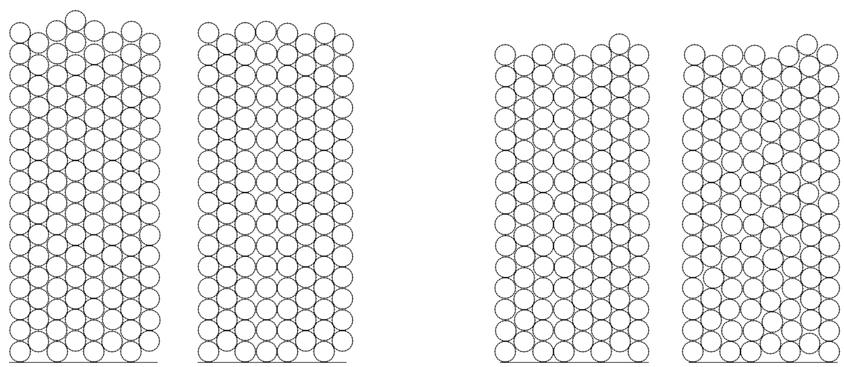

Fig. 3. There is a transition from the first to the second configuration when T_b gets sufficiently small: a column slides down. When T_b starts increasing again this column eventually recovers its original height, but at a higher value of T_b than before (hence hysteresis). The transition from the third to the fourth configurations is more subtle, because there is a defect from the start and nearby columns abandon their straight configurations adopting a zig-zag one for lower temperatures. Crystallographic order is abandoned because the system is too cold.

The discontinuities in the function $h(T_b)$ are rearrangement (topological) transitions and they are described in the caption of Fig. 3. They are meaningful only because the system is quite finite. In fact, one can argue that in a quasi-elastic limit where $N \to \infty$ and the energy loss per collision tends to zero in such a way that, say, the granular temperature has roughly the same profile, these transitions, measured as a discontinuity of h/σ would vanish. The topological transitions themselves would continue being there but one would have to characterize them in a different way.

Transitions where a column simply suffers a translation imply a jump in h of order $O(N_y/N)$ where N_y is the number of particles in the falling column. This type of transition is illustrated by the two states at left in Fig. 3. Transitions in which crystalline order changes to a local zig-zag configuration represent a much smaller change in h. This last transition is peculiar and perhaps counter-intuitive because the colder configuration has less symmetry than the warmer one. This type of transition is illustrated by the two states at right in Fig. 3. Both transitions are quite small and probably difficult to observe experimentally.

Something like an entropy. In these systems the gravitational potential energy is the dominant component of the energy. The particles keep on average a small distance between them. The distance does not vanish because the particles are vibrating as a product of the steady (vibrational) energy input from the base. This rattling plays the role of a repulsive potential between the particles and gives rise to a small area (volume in 3D) available to each particle. An estimate of "the number of configurations" is the product of all these areas (it cannot be a simple product because particles are highly correlated) and therefore something like an entropy, in the spirit of Edwards (Edwards et al.) could be defined through the logarithm of such product.

But there is a connection with ordinary statistical mechanics because similar rearrangement transitions can be observed in conservative systems with homogeneous temperature. We have checked this performing a Monte Carlo Metropolis canonical simulation of a system of hard disks with a weak repulsive potential and compactified in a box due to their own weight. The result has been that the almost perfectly compactified system kept slowly cooling down does suffers a sudden change in the height of the center of mass and when the system is warmed back it shows a hysteretic cycle just as the granular systems have been shown to present.

Acknowledgment This work has been partially financed by *Fondecyt* research grant 1030993 and *Fondap* grant 11980002. We also thank CIMAT for its computational facilities.

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